Monte Carlo Simulations to Model Flux Decline in Dead-End Microfiltration Operations

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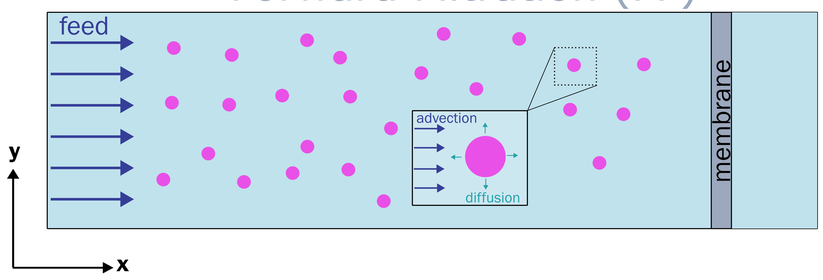
OBJECTIVES

(1) Draw from classical membrane filtration theory to develop a Monte Carlo code built on physical, real-world parameters to capture flux decline and recovery in dead-end membrane filtration.

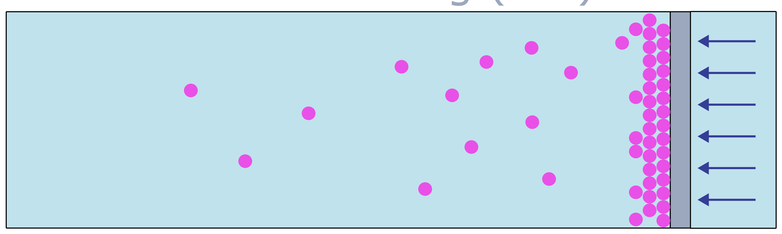
(2) Explore how varying backwashing parameters (frequency, flow rate, etc.) affects flux recovery and implement fitting algorithms to estimate unknown parameter values.

FILTRATION PHASES

Forward Filtration (FF)



Backwashing (BW)



MODEL

Foulant transport is modeled as a stochastic advection-diffusion equation:

$$dX(t) = J(t)\,dt + \sqrt{2\kappa}\,dW(t)$$
$$dY(t) = \sqrt{2\kappa}\,dW(t)$$

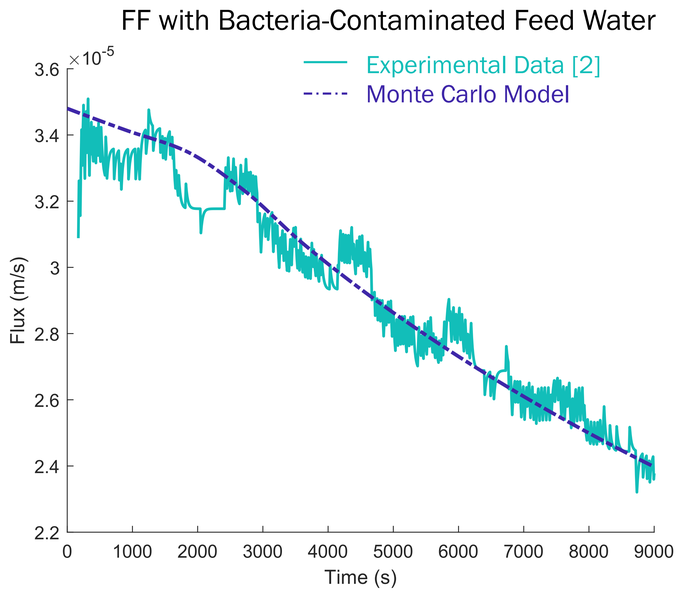
$X(t), Y(t)$: position of particle at time t [m]
$J(t)$: axial flux [m/s]
κ : diffusion coefficient [m^2/s]
$dW(t)$: 1D Brownian motion [$s^{1/2}$]
t : time [s]

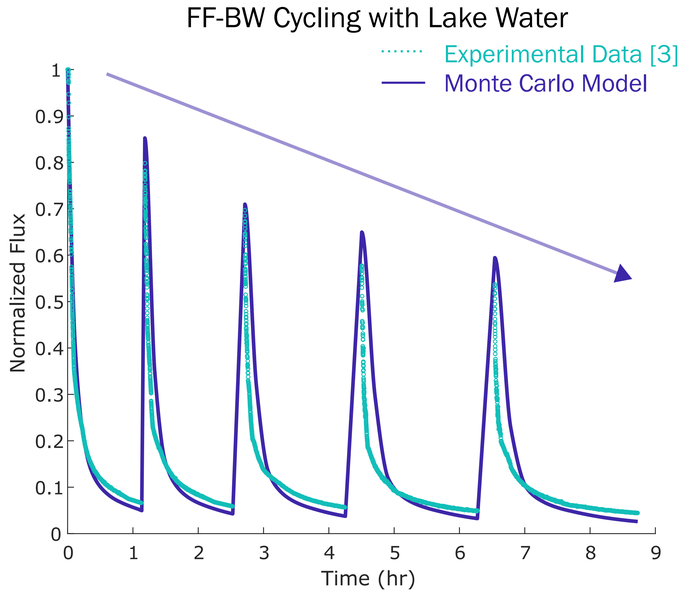
Flux is calculated throughout the simulations according to our equation adapted from classical filtration theory [1] to integrate experimental parameters:

$$J(t) = \frac{J_0}{1 + J_0 \cdot \frac{F_{\text{conc}}}{n} \cdot F_{\text{area}} \cdot A_{\text{adj}} \cdot B_{\text{gr}}(t)}$$

J_0 : initial flux [m/s]
F_{conc} : concentration of foulants in feed [cells/m^3]
n : foulant input rate [cells/s]
F_{area} : cross-sectional area of single foulant [m^2/cell]
A_{adj} : non-physical parameter fit to experimental data [-]
F_{gr} : # of foulants on the membrane [cells]

RESULTS: FLUX DECLINE AND RECOVERY





Backwashing cleans the membrane to recover some of the flux lost during forward filtration, but not all of it. Thus, the flux follows a downward trend overall.

FUTURE WORK

(1) Simulate FF-BW cycles of contaminated water containing foulants with multiple particle sizes.
(2) Extend from 2D to 3D to visualize cake formation at the membrane.

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[1] Bowen et al., *Journal of Membrane Science*, 1995.
[2] Xu & Chellam, *Environmental Science & Technology*, 2005.
[3] Gamage & Chellam, *Environmental Science & Technology*, 2014.